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(2,9-Dimethoxy-1,10-phenanthroline-κ^2N,N')nitratosilver(I)

Xin-Sheng Wan, Hai-Yan Zhang, Cao-Yuan Niu,* Chun-Hong Kou and Cao-Ling Feng

College of Sciences, Henan Agricultural University, Zhengzhou 450002, People's Republic of China
Correspondence e-mail: niu_cy2000@yahoo.com.cn

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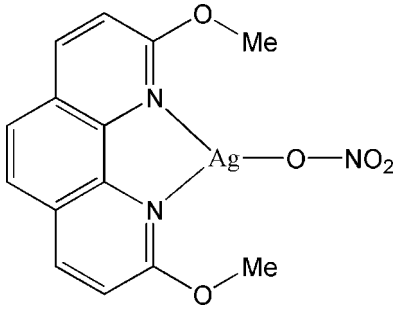
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.122; data-to-parameter ratio = 12.7.

In the crystal structure of the title compound, $[Ag(NO_3)(C_{14}H_{12}N_2O_2)]$, the Ag^I centre is three-coordinated by two N atoms from 2,9-dimethoxy-1,10-phenanthroline and one O atom of the nitrate anion. The Ag—N bond lengths are almost identical, and O—Ag—N bond angles are larger than the bite angle N—Ag—N. In the main ligand, the O and C atoms of the methoxy groups lie almost in the plane defined by the phenanthroline ring system. Based on the extended delocalized π system of phenanthroline and the d^{10} electronic configuration of the metal centre, the title complex is expected to produce strong luminescent emission when properly excited.

Related literature

For related literature about Ag^I luminescent complexes, see: Bie *et al.* (2006); Majumder *et al.* (2006); For the synthesis of 2,9-dimethoxy-1,10-phenanthroline, see: Pijper *et al.* (1984).



Experimental

Crystal data

$[Ag(NO_3)(C_{14}H_{12}N_2O_2)]$
M_r = 410.14
Triclinic, $P\overline{1}$
a = 6.8510 (12) Å
b = 10.3094 (17) Å
c = 10.7294 (18) Å
α = 105.174 (3)°
β = 92.224 (3)°
γ = 92.896 (3)°
V = 729.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.41 mm^{-1}
T = 291 (2) K
0.50 × 0.30 × 0.11 mm

Data collection

Bruker APEX-II CCD detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.539, T_{max} = 0.860
3810 measured reflections
2659 independent reflections
2271 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.122
S = 1.07
2659 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.309 (3)	Ag1—O2	2.214 (4)
Ag1—N2	2.316 (3)		
O2—Ag1—N1	144.53 (13)	N1—Ag1—N2	72.42 (11)
O2—Ag1—N2	142.80 (13)		

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2139).

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supplementary materials

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(2,9-Dimethoxy-1,10-phenanthroline-κ^2N,N')nitratosilver(I)

X.-S. Wan, H.-Y. Zhang, C.-Y. Niu, C.-H. Kou and C.-L. Feng

Comment

2,9-Dimethoxy-1,10-phenanthroline and 2,9-diethoxy-1,10-phenanthroline were synthesized at early time and they are known to possess antimycoplasmal activity in the presence of copper (Pijper *et al.*, 1984). However, crystal structures of their coordination complexes with transition metal ions have not been reported so far.

The title compound, (I), is a mononuclear Ag^I complex of 2,9-dimethoxy-1,10-phenanthroline (Fig.1). The Ag metal centre is three coordinated by two N atoms from the 1,10-phenanthroline ring and one O atom from the nitrate anion. The Ag—O bond length is 2.214 (4) Å, and the Ag—N bond lengths are 2.309 (3) and 2.316 (3) Å. The O—Ag—N bond angles are 142.80 (13) and 144.53 (13)°, which are larger than N—Ag—N angle. Intermolecular interactions corresponding to π–π stacking contacts between phenanthroline rings are observed in the crystal structure, with separations of *ca*. 3.5 Å. Regarding the main ligand, it remains almost planar, with the O and C atoms of methoxy groups deviating from the phenanthroline plane by about 0.03 and 0.18 Å, respectively.

Because the ligand 1,10-phenanthroline was reported to be used in the preparation of some potentially strong luminescent materials with d^{10} metals, it can be expected that the title complex also has strong luminescent properties (Majumder *et al.*, 2006; Bie *et al.*, 2006).

Experimental

The organic ligand 2,9-dimethoxy-1,10-phenanthroline was prepared according to the literature procedure (Pijper *et al.*, 1984). The slow evaporation of a mixture of the ligand (0.024 g, 0.1 mmol) and silver nitrate (0.017 g, 0.1 mmol) in methanol (30 ml) afforded colourless needles suitable for X-ray crystallography in about 7 days (yield: 40%).

Refinement

C-bound H atoms in phenanthroline ring and methyl groups were placed at calculated positions (C—H = 0.93 Å and 0.96 Å, respectively), and they were included in the refinement in the riding-model approximation, with U_{iso}(H) values set at 1.2 times and 1.5 times U_{eq}(C), respectively. The final difference map had a highest peak at 0.93 Å from atom Ag1 and a deepest hole at 0.85 Å from atom Ag1, but was otherwise featureless.

Figures

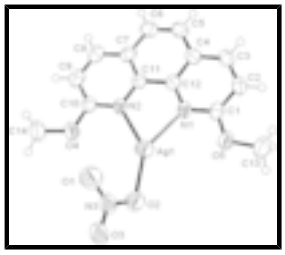


Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

(2,9-Dimethoxy-1,10-phenanthroline-κ^2*N*,*N*')nitratosilver(I)

Crystal data

$[Ag(NO_3)(C_{14}H_{12}N_2O_2)]$	$Z = 2$
$M_r = 410.14$	$F_{000} = 408$
Triclinic, $P\overline{1}$	$D_x = 1.867$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.8510$ (12) Å	Cell parameters from 1736 reflections
$b = 10.3094$ (17) Å	$\theta = 3.0$–25.5°
$c = 10.7294$ (18) Å	$\mu = 1.41$ mm^{-1}
$\alpha = 105.174$ (3)°	$T = 291$ (2) K
$\beta = 92.224$ (3)°	Needle, colourless
$\gamma = 92.896$ (3)°	0.50 × 0.30 × 0.11 mm
$V = 729.4$ (2) Å^3	

Data collection

Bruker APEX-II CCD detector diffractometer	2659 independent reflections
Radiation source: fine-focus sealed tube	2271 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.015$
$T = 291(2)$ K	$\theta_{max} = 25.5^\circ$
φ and ω scans	$\theta_{min} = 3.0^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -8\rightarrow7$
$T_{min} = 0.539$, $T_{max} = 0.860$	$k = -9\rightarrow12$
3810 measured reflections	$l = -12\rightarrow12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.122$	$w = 1/[\sigma^2(F_o^2) + (0.0759P)^2 + 0.3168P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
2659 reflections	$\Delta\rho_{max} = 1.51$ e Å^{-3}
210 parameters	$\Delta\rho_{min} = -0.65$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.21110 (6)	0.31461 (3)	0.64007 (3)	0.05986 (19)
O1	0.3742 (7)	0.2845 (5)	0.8828 (4)	0.0870 (13)
O2	0.1719 (7)	0.1546 (4)	0.7418 (4)	0.0807 (12)
O3	0.2569 (8)	0.0994 (4)	0.9147 (3)	0.0861 (14)
O4	0.1377 (5)	0.5804 (3)	0.8756 (3)	0.0524 (8)
O5	0.2725 (5)	0.1390 (3)	0.3440 (3)	0.0558 (8)
N1	0.2584 (5)	0.3565 (3)	0.4420 (3)	0.0381 (7)
N2	0.1984 (4)	0.5443 (3)	0.6671 (3)	0.0361 (7)
N3	0.2718 (6)	0.1797 (4)	0.8481 (3)	0.0550 (10)
C1	0.2876 (6)	0.2654 (4)	0.3324 (4)	0.0428 (9)
C2	0.3284 (6)	0.2990 (5)	0.2166 (4)	0.0462 (10)
H2	0.3477	0.2327	0.1414	0.055*
C3	0.3388 (6)	0.4321 (5)	0.2181 (4)	0.0492 (10)
H3	0.3669	0.4568	0.1430	0.059*
C4	0.3077 (6)	0.5324 (5)	0.3314 (4)	0.0430 (9)
C5	0.3116 (7)	0.6722 (5)	0.3377 (4)	0.0540 (11)
H5	0.3367	0.7005	0.2640	0.065*
C6	0.2793 (8)	0.7641 (5)	0.4488 (5)	0.0558 (11)
H6	0.2828	0.8549	0.4506	0.067*
C7	0.2401 (6)	0.7249 (4)	0.5630 (4)	0.0444 (9)
C8	0.2094 (6)	0.8164 (4)	0.6822 (5)	0.0499 (10)
H8	0.2114	0.9080	0.6877	0.060*
C9	0.1771 (6)	0.7737 (4)	0.7882 (4)	0.0476 (10)
H9	0.1590	0.8348	0.8670	0.057*
C10	0.1713 (6)	0.6350 (4)	0.7773 (4)	0.0405 (9)
C11	0.2338 (5)	0.5881 (4)	0.5614 (4)	0.0353 (8)
C12	0.2668 (5)	0.4886 (4)	0.4419 (4)	0.0370 (8)
C13	0.2794 (9)	0.0303 (5)	0.2287 (5)	0.0701 (15)
H13A	0.1730	0.0342	0.1692	0.105*
H13B	0.2686	−0.0541	0.2508	0.105*
H13C	0.4013	0.0383	0.1893	0.105*
C14	0.1242 (8)	0.6691 (6)	1.0025 (5)	0.0644 (13)
H14A	0.2473	0.7191	1.0299	0.097*
H14B	0.0923	0.6171	1.0620	0.097*
H14C	0.0239	0.7303	1.0002	0.097*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0811 (3)	0.0493 (3)	0.0537 (3)	0.00036 (19)	−0.00120 (19)	0.02297 (18)
O1	0.081 (3)	0.101 (3)	0.076 (3)	−0.022 (2)	−0.002 (2)	0.024 (2)
O2	0.136 (4)	0.051 (2)	0.057 (2)	−0.008 (2)	−0.016 (2)	0.0224 (17)
O3	0.164 (4)	0.055 (2)	0.0444 (19)	0.020 (2)	0.005 (2)	0.0189 (17)
O4	0.0637 (19)	0.0552 (19)	0.0365 (15)	0.0055 (15)	0.0068 (13)	0.0078 (13)
O5	0.075 (2)	0.0411 (16)	0.0458 (17)	0.0042 (15)	0.0011 (15)	0.0020 (13)
N1	0.0361 (17)	0.0416 (18)	0.0326 (16)	0.0007 (14)	−0.0027 (13)	0.0040 (13)
N2	0.0326 (16)	0.0376 (17)	0.0352 (16)	0.0008 (13)	−0.0004 (12)	0.0049 (13)
N3	0.076 (3)	0.046 (2)	0.043 (2)	0.016 (2)	0.0104 (19)	0.0083 (18)
C1	0.039 (2)	0.045 (2)	0.040 (2)	0.0040 (17)	−0.0024 (16)	0.0044 (17)
C2	0.045 (2)	0.055 (3)	0.0325 (19)	0.0038 (19)	0.0004 (16)	0.0006 (18)
C3	0.044 (2)	0.067 (3)	0.035 (2)	−0.001 (2)	−0.0003 (17)	0.0120 (19)
C4	0.036 (2)	0.053 (2)	0.041 (2)	−0.0004 (17)	−0.0030 (16)	0.0147 (18)
C5	0.060 (3)	0.059 (3)	0.046 (2)	−0.007 (2)	−0.004 (2)	0.023 (2)
C6	0.071 (3)	0.046 (3)	0.055 (3)	−0.001 (2)	−0.002 (2)	0.023 (2)
C7	0.040 (2)	0.045 (2)	0.048 (2)	−0.0023 (17)	−0.0054 (17)	0.0138 (18)
C8	0.053 (3)	0.037 (2)	0.056 (2)	0.0044 (19)	0.000 (2)	0.0050 (18)
C9	0.046 (2)	0.044 (2)	0.047 (2)	0.0046 (18)	0.0002 (18)	0.0023 (18)
C10	0.035 (2)	0.044 (2)	0.041 (2)	0.0010 (16)	−0.0006 (16)	0.0082 (17)
C11	0.0312 (18)	0.038 (2)	0.0363 (19)	0.0019 (15)	−0.0020 (14)	0.0101 (15)
C12	0.0287 (18)	0.045 (2)	0.0371 (19)	−0.0002 (15)	−0.0043 (15)	0.0106 (16)
C13	0.093 (4)	0.048 (3)	0.061 (3)	0.007 (3)	0.004 (3)	0.000 (2)
C14	0.075 (3)	0.071 (3)	0.042 (2)	0.005 (3)	0.006 (2)	0.005 (2)

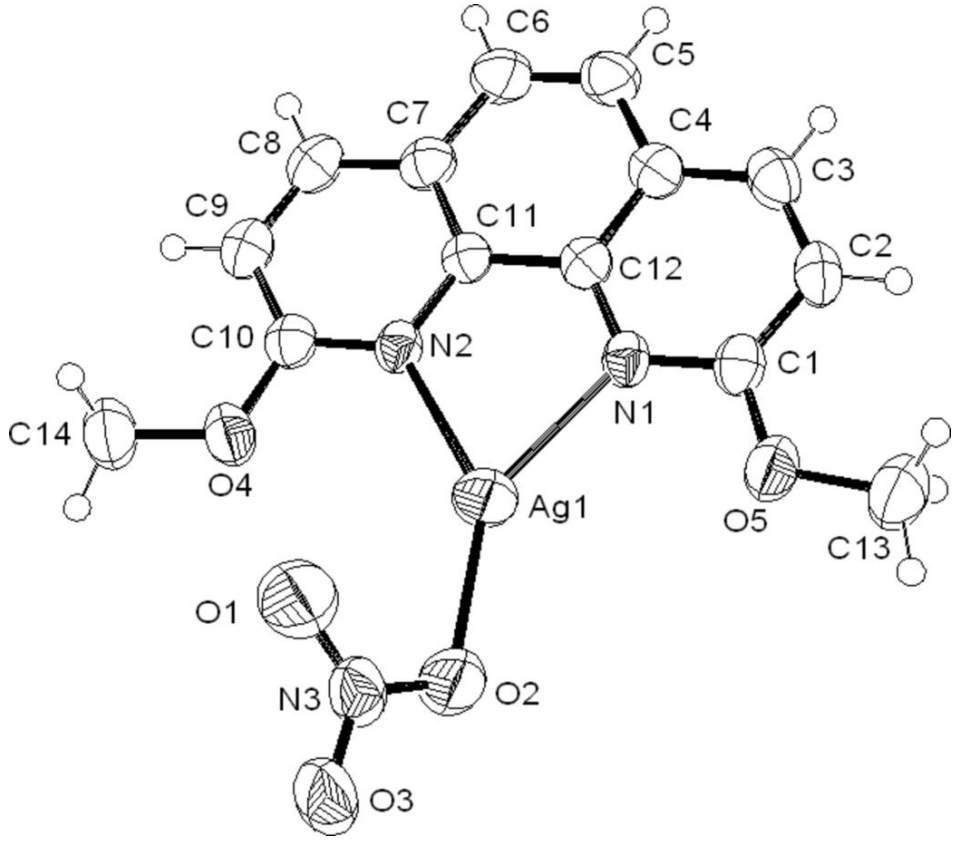
Geometric parameters (Å, °)

Ag1—N1	2.309 (3)	C4—C12	1.407 (6)
Ag1—N2	2.316 (3)	C4—C5	1.424 (6)
Ag1—O2	2.214 (4)	C5—C6	1.349 (7)
O1—N3	1.221 (5)	C5—H5	0.9300
O2—N3	1.266 (5)	C6—C7	1.418 (7)
O3—N3	1.230 (5)	C6—H6	0.9300
O4—C10	1.341 (5)	C7—C11	1.404 (6)
O4—C14	1.437 (5)	C7—C8	1.407 (6)
O5—C1	1.340 (6)	C8—C9	1.345 (7)
O5—C13	1.440 (5)	C8—H8	0.9300
N1—C1	1.328 (5)	C9—C10	1.402 (6)
N1—C12	1.361 (5)	C9—H9	0.9300
N2—C10	1.327 (5)	C11—C12	1.451 (5)
N2—C11	1.353 (5)	C13—H13A	0.9600
C1—C2	1.409 (6)	C13—H13B	0.9600
C2—C3	1.366 (6)	C13—H13C	0.9600
C2—H2	0.9300	C14—H14A	0.9600
C3—C4	1.406 (6)	C14—H14B	0.9600
C3—H3	0.9300	C14—H14C	0.9600

O2—Ag1—N1	144.53 (13)	C7—C6—H6	119.4
O2—Ag1—N2	142.80 (13)	C11—C7—C8	116.4 (4)
N1—Ag1—N2	72.42 (11)	C11—C7—C6	119.9 (4)
N3—O2—Ag1	113.0 (3)	C8—C7—C6	123.7 (4)
C10—O4—C14	118.3 (4)	C9—C8—C7	121.1 (4)
C1—O5—C13	118.1 (4)	C9—C8—H8	119.4
C1—N1—C12	118.3 (3)	C7—C8—H8	119.4
C1—N1—Ag1	126.2 (3)	C8—C9—C10	118.6 (4)
C12—N1—Ag1	115.4 (2)	C8—C9—H9	120.7
C10—N2—C11	118.4 (3)	C10—C9—H9	120.7
C10—N2—Ag1	125.9 (3)	N2—C10—O4	113.3 (4)
C11—N2—Ag1	115.6 (2)	N2—C10—C9	122.8 (4)
O1—N3—O3	122.4 (5)	O4—C10—C9	124.0 (4)
O1—N3—O2	119.0 (4)	N2—C11—C7	122.8 (4)
O3—N3—O2	118.6 (4)	N2—C11—C12	118.0 (3)
N1—C1—O5	112.8 (4)	C7—C11—C12	119.2 (4)
N1—C1—C2	123.2 (4)	N1—C12—C4	122.8 (4)
O5—C1—C2	124.0 (4)	N1—C12—C11	118.3 (3)
C3—C2—C1	118.0 (4)	C4—C12—C11	118.9 (4)
C3—C2—H2	121.0	O5—C13—H13A	109.5
C1—C2—H2	121.0	O5—C13—H13B	109.5
C2—C3—C4	121.0 (4)	H13A—C13—H13B	109.5
C2—C3—H3	119.5	O5—C13—H13C	109.5
C4—C3—H3	119.5	H13A—C13—H13C	109.5
C3—C4—C12	116.7 (4)	H13B—C13—H13C	109.5
C3—C4—C5	123.4 (4)	O4—C14—H14A	109.5
C12—C4—C5	119.9 (4)	O4—C14—H14B	109.5
C6—C5—C4	120.9 (4)	H14A—C14—H14B	109.5
C6—C5—H5	119.5	O4—C14—H14C	109.5
C4—C5—H5	119.5	H14A—C14—H14C	109.5
C5—C6—C7	121.2 (4)	H14B—C14—H14C	109.5
C5—C6—H6	119.4		
N1—Ag1—O2—N3	135.9 (3)	C7—C8—C9—C10	−1.1 (7)
N2—Ag1—O2—N3	−52.8 (5)	C11—N2—C10—O4	−179.9 (3)
O2—Ag1—N1—C1	−5.5 (5)	Ag1—N2—C10—O4	−4.2 (5)
N2—Ag1—N1—C1	−180.0 (3)	C11—N2—C10—C9	0.3 (6)
O2—Ag1—N1—C12	178.2 (3)	Ag1—N2—C10—C9	176.0 (3)
N2—Ag1—N1—C12	3.7 (2)	C14—O4—C10—N2	174.3 (4)
O2—Ag1—N2—C10	6.1 (4)	C14—O4—C10—C9	−5.9 (6)
N1—Ag1—N2—C10	−179.2 (3)	C8—C9—C10—N2	0.7 (6)
O2—Ag1—N2—C11	−178.0 (3)	C8—C9—C10—O4	−179.0 (4)
N1—Ag1—N2—C11	−3.4 (2)	C10—N2—C11—C7	−1.0 (5)
Ag1—O2—N3—O1	0.3 (6)	Ag1—N2—C11—C7	−177.1 (3)
Ag1—O2—N3—O3	177.9 (4)	C10—N2—C11—C12	178.9 (3)
C12—N1—C1—O5	−179.0 (3)	Ag1—N2—C11—C12	2.7 (4)
Ag1—N1—C1—O5	4.8 (5)	C8—C7—C11—N2	0.6 (6)
C12—N1—C1—C2	0.6 (6)	C6—C7—C11—N2	179.6 (4)
Ag1—N1—C1—C2	−175.6 (3)	C8—C7—C11—C12	−179.2 (4)

C13—O5—C1—N1	173.2 (4)	C6—C7—C11—C12	−0.2 (6)
C13—O5—C1—C2	−6.3 (7)	C1—N1—C12—C4	−0.9 (5)
N1—C1—C2—C3	0.2 (6)	Ag1—N1—C12—C4	175.7 (3)
O5—C1—C2—C3	179.7 (4)	C1—N1—C12—C11	179.6 (3)
C1—C2—C3—C4	−0.7 (6)	Ag1—N1—C12—C11	−3.8 (4)
C2—C3—C4—C12	0.3 (6)	C3—C4—C12—N1	0.5 (6)
C2—C3—C4—C5	−178.3 (4)	C5—C4—C12—N1	179.1 (4)
C3—C4—C5—C6	179.5 (4)	C3—C4—C12—C11	179.9 (4)
C12—C4—C5—C6	0.9 (7)	C5—C4—C12—C11	−1.4 (5)
C4—C5—C6—C7	−0.1 (8)	N2—C11—C12—N1	0.7 (5)
C5—C6—C7—C11	−0.2 (7)	C7—C11—C12—N1	−179.4 (3)
C5—C6—C7—C8	178.6 (4)	N2—C11—C12—C4	−178.8 (3)
C11—C7—C8—C9	0.4 (6)	C7—C11—C12—C4	1.1 (5)
C6—C7—C8—C9	−178.5 (4)		

Fig. 1


C6
C5
C7
C4
C8
C3
C9
C11
C2
C12
C10
N2
C1
N1
C14
O4
Ag1
O5
C13
O1
N3
O2
O3